Nathan A Baker

List of Publications by Year
in descending order

119 papers	18,037 citations	61984 43 h-index	34986 98 g-index
124 all docs	124 docs citations	124 times ranked	22906 citing authors

#	Article	IF	Citations
1	Electrostatics of nanosystems: Application to microtubules and the ribosome. Proceedings of the National Academy of Sciences of the United States of America, 2001, 98, 10037-10041.	7.1	6,623
2	PDB2PQR: an automated pipeline for the setup of Poisson-Boltzmann electrostatics calculations. Nucleic Acids Research, 2004, 32, W665-W667.	14.5	3,014
3	PDB2PQR: expanding and upgrading automated preparation of biomolecular structures for molecular simulations. Nucleic Acids Research, 2007, 35, W522-W525.	14.5	1,659
4	Improvements to the <scp>APBS</scp> biomolecular solvation software suite. Protein Science, 2018, 27, 112-128.	7.6	1,399
5	Improving implicit solvent simulations: a Poisson-centric view. Current Opinion in Structural Biology, 2005, 15, 137-143.	5.7	322
6	Assessing implicit models for nonpolar mean solvation forces: The importance of dispersion and volume terms. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 8331-8336.	7.1	270
7	Adaptive multilevel finite element solution of the Poisson-Boltzmann equation I. Algorithms and examples. Journal of Computational Chemistry, 2000, 21, 1319-1342.	3.3	255
8	Web servers and services for electrostatics calculations with APBS and PDB2PQR. Journal of Computational Chemistry, 2011, 32, 1488-1491.	3.3	254
9	Progress in the prediction of pK_a values in proteins. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3260-3275.	2.6	229
10	Poissonâ€“Boltzmann Methods for Biomolecular Electrostatics. Methods in Enzymology, 2004, 383, 94-118.	1.0	182
11	Adaptive multilevel finite element solution of the Poisson-Boltzmann equation II. Refinement at solvent-accessible surfaces in biomolecular systems. Journal of Computational Chemistry, 2000, 21, 1343-1352.	3.3	169
12	Biomolecular electrostatics and solvation: a computational perspective. Quarterly Reviews of Biophysics, 2012, 45, 427-491.	5.7	152
13	A multiscale model linking ion-channel molecular dynamics and electrostatics to the cardiac action potential. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 11102-11106.	7.1	124
14	The physical basis of microtubule structure and stability. Protein Science, 2009, 12, 2257-2261.	7.6	123
15	Differential geometry based solvation model I: Eulerian formulation. Journal of Computational Physics, 2010, 229, 8231-8258.	3.8	110
16	Molecular Dynamics Simulations of Asymmetric NaCl and KCl Solutions Separated by Phosphatidylcholine Bilayers: Potential Drops and Structural Changes Induced by Strong Na+-Lipid Interactions and Finite Size Effects. Biophysical Journal, 2008, 94, 3565-3576.	0.5	106
17	Data-driven parameterization of the generalized Langevin equation. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 14183-14188.	7.1	103
18	NanoParticle Ontology for cancer nanotechnology research. Journal of Biomedical Informatics, 2011, 44, 59-74.	4.3	96

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19	Solvation forces on biomolecular structures: A comparison of explicit solvent and Poisson-Boltzmann models. Journal of Computational Chemistry, 2004, 25, 1623-1629.	3.3	92
20	APBSmem: A Graphical Interface for Electrostatic Calculations at the Membrane. PLoS ONE, 2010, 5, e12722.	2.5	83
21	Finite Element Solution of the Steady-State Smoluchowski Equation for Rate Constant Calculations. Biophysical Journal, 2004, 86, 2017-2029.	0.5	81
22	Polarizable atomic multipole solutes in a Poisson-Boltzmann continuum. Journal of Chemical Physics, 2007, 126, 124114.	3.0	79
23	Molecular Recognition by Cholesterol Esterase of Active Site Ligands:Â Structureâ˜Reactivity Effects for Inhibition by Aryl Carbamates and Subsequent Carbamylenzyme Turnoverâ€. Biochemistry, 1996, 35, 16723-16734.	2.5	78
24	Perturbations of Membrane Structure by Cholesterol and Cholesterol Derivatives Are Determined by Sterol Orientation. Journal of the American Chemical Society, 2009, 131, 4854-4865.	13.7	77
25	ISA-TAB-Nano: A Specification for Sharing Nanomaterial Research Data in Spreadsheet-based Format. BMC Biotechnology, 2013, 13, 2.	3.3	72
26	Why double-stranded RNA resists condensation. Nucleic Acids Research, 2014, 42, 10823-10831.	14.5	67
27	Bridging Implicit and Explicit Solvent Approaches for Membrane Electrostatics. Biophysical Journal, 2002, 83, 1374-1379.	0.5	66
28	Computational Methods for Biomolecular Electrostatics. Methods in Cell Biology, 2008, 84, 843-870.	1.1	65
29	Molecular Dynamics Simulation of the Escherichia coli NikR Protein: Equilibrium Conformational Fluctuations Reveal Interdomain Allosteric Communication Pathways. Journal of Molecular Biology, 2008, 378, 1155-1173.	4.2	63
30	Electrostatic properties of cowpea chlorotic mottle virus and cucumber mosaic virus capsids. Biopolymers, 2006, 82, 106-120.	2.4	59
31	Differential geometry based solvation model II: Lagrangian formulation. Journal of Mathematical Biology, 2011, 63, 1139-1200.	1.9	58
32	Application of a hemolysis assay for analysis of complement activation by perfluorocarbon nanoparticles. Nanomedicine: Nanotechnology, Biology, and Medicine, 2014, 10, 651-660.	3.3	55
33	Finite Element Simulations of Acetylcholine Diffusion in Neuromuscular Junctions. Biophysical Journal, 2003, 84, 2234-2241.	0.5	54
34	Electrostatic interaction between RNA and protein capsid in cowpea chlorotic mottle virus simulated by a coarse-grain RNA model and a Monte Carlo approach. Biopolymers, 2004, 75, 325-337.	2.4	54
35	iAPBS: a programming interface to the adaptive Poissonâ€“Boltzmann solver. Computational Science & Discovery, 2012, 5, 015005.	1.5	53
36	Binding of Aminoglycoside Antibiotics to the Small Ribosomal Subunit:Â A Continuum Electrostatics Investigation. Journal of the American Chemical Society, 2002, 124, 1438-1442.	13.7	52

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37	25-Hydroxycholesterol Increases the Availability of Cholesterol in Phospholipid Membranes. Biophysical Journal, 2011, 100, 948-956.	0.5	50
38	Simulations of RNA Interactions with Monovalent Ions. Methods in Enzymology, 2009, 469, 411-432.	1.0	48
39	Improved Coarse-Grained Modeling of Cholesterol-Containing Lipid Bilayers. Journal of Chemical Theory and Computation, 2014, 10, 2137-2150.	5.3	48
40	Spermine Condenses DNA, but Not RNA Duplexes. Biophysical Journal, 2017, 112, 22-30.	0.5	48
41	Opposing Effects of Multivalent Ions on the Flexibility of DNA and RNA. Physical Review Letters, 2016, 117, 028101.	7.8	47
42	Side-chain oxysterols: From cells to membranes to molecules. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 330-336.	2.6	46
43	The Structural Basis of Cholesterol Accessibility in Membranes. Biophysical Journal, 2013, 105, 1838-1847.	0.5	46
44	Molecular Dynamics Simulations of Salicylate Effects on the Micro- and Mesoscopic Properties of a Dipalmitoylphosphatidylcholine Bilayer. Biochemistry, 2005, 44, 13425-13438.	2.5	44
45	Optimizing the Poisson Dielectric Boundary with Explicit Solvent Forces and Energies:â€‰ Lessons Learned with Atom-Centered Dielectric Functions. Journal of Chemical Theory and Computation, 2007, 3, 170-183.	5.3	42
46	Variational approach for nonpolar solvation analysis. Journal of Chemical Physics, 2012, 137, 084101.	3.0	40
47	Enhancing sparsity of Hermite polynomial expansions by iterative rotations. Journal of Computational Physics, 2016, 307, 94-109.	3.8	39
48	Delineation and Decomposition of Energies Involved in Quaternary Ammonium Binding in the Active Site of Acetylcholinesterase. Journal of the American Chemical Society, 2000, 122, 2975-2980.	13.7	37
49	Continuum Diffusion Reaction Rate Calculations of Wild-Type and Mutant Mouse Acetylcholinesterase: Adaptive Finite Element Analysis. Biophysical Journal, 2004, 87, 1558-1566.	0.5	37
50	Biomolecular Applications of Poisson-Boltzmann Methods. Reviews in Computational Chemistry, 2005, , 349-379.	1.5	36
51	Solvent reaction field potential inside an uncharged globular protein: A bridge between implicit and explicit solvent models?. Journal of Chemical Physics, 2007, 127, 155101.	3.0	36
52	Informatics and standards for nanomedicine technology. Wiley Interdisciplinary Reviews: Nanomedicine and Nanobiotechnology, 2011, 3, 511-532.	6.1	36
53	How Much Chemistry Does a Deep Neural Network Need to Know to Make Accurate Predictions?. , 2018, , .		35
54	Polarization around an ion in a dielectric continuum with truncated electrostatic interactions. Journal of Chemical Physics, 1999, 110, 10679-10692.	3.0	34

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55	Finite Element Analysis of the Time-Dependent Smoluchowski Equation for Acetylcholinesterase Reaction Rate Calculations. Biophysical Journal, 2007, 92, 3397-3406.	0.5	33
56	The Role of Correlation and Solvation in Ion Interactions with B-DNA. Biophysical Journal, 2016, 110, 315-326.	0.5	33
57	Application of New Multiresolution Methods for the Comparison of Biomolecular Electrostatic Properties in the Absence of Global Structural Similarity. Multiscale Modeling and Simulation, 2006, 5, 1196-1213.	1.6	32
58	Tetrameric Mouse Acetylcholinesterase: Continuum Diffusion Rate Calculations by Solving the Steady-State Smoluchowski Equation Using Finite Element Methods. Biophysical Journal, 2005, 88, 1659-1665.	0.5	31
59	Visualizing biomolecular electrostatics in virtual reality with UnityMolâ€APBS. Protein Science, 2020, 29, 237-246.	7.6	31
60	Side-Chain Oxysterols Modulate Cholesterol Accessibility through Membrane Remodeling. Biochemistry, 2014, 53, 3042-3051.	2.5	30
61	Comparative hazard analysis and toxicological modeling of diverse nanomaterials using the embryonic zebrafish (EZ) metric of toxicity. Journal of Nanoparticle Research, 2015, 17, 250.	1.9	30
62	Iron Responsive Element RNA Flexibility Described by NMR and Isotropic Reorientational Eigenmode Dynamics. Journal of Biomolecular NMR, 2005, 32, 179-193.	2.8	29
63	Implicit Solvent Electrostatics in Biomolecular Simulation. , 2006, , 263-295.		29
64	Constructing Surrogate Models of Complex Systems with Enhanced Sparsity: Quantifying the Influence of Conformational Uncertainty in Biomolecular Solvation. Multiscale Modeling and Simulation, 2015, 13, 1327-1353.	1.6	27
65	Continuum Electrostatics Approaches to Calculating pKas and Ems in Proteins. Methods in Enzymology, 2016, 578, 1-20.	1.0	27
66	Interaction of Melittin Peptides with Perfluorocarbon Nanoemulsion Particles. Journal of Physical Chemistry B, 2011, 115, 15271-15279.	2.6	24
67	Probing 3â€²-ssDNA Loop Formation in E. coli RecBCD/RecBCâ€“DNA Complexes Using Non-natural DNA: A Model for â€œChiâ€•Recognition Complexes. Journal of Molecular Biology, 2006, 362, 26-43.	4.2	22
68	Simulation of fusion-mediated nanoemulsion interactions with model lipid bilayers. Soft Matter, 2012, 8, 7024.	2.7	22
69	ISIM: A Program for Grand Canonical Monte Carlo Simulations of the Ionic Environment of Biomolecules. Molecular Simulation, 2004, 30, 45-61.	2.0	21
70	Parameterization of a geometric flow implicit solvation model. Journal of Computational Chemistry, 2013, 34, 687-695.	3.3	21
71	Data-driven molecular modeling with the generalized Langevin equation. Journal of Computational Physics, 2020, 418, 109633.	3.8	21
72	On the development of protein pK_a calculation algorithms. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3287-3298.	2.6	19

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73	Standardizing data. Nature Nanotechnology, 2013, 8, 73-74.	31.5	19
74	Assessing the performance of implicit solvation models at a nucleic acid surface. Physical Chemistry Chemical Physics, 2008, 10, 4889.	2.8	18
75	Theoretical and experimental investigations of electrostatic effects on acetylcholinesterase catalysis and inhibition. Chemico-Biological Interactions, 1999, 119-120, 99-110.	4.0	16
76	Toward Quantum Computing for High-Energy Excited States in Molecular Systems: Quantum Phase Estimations of Core-Level States. Journal of Chemical Theory and Computation, 2021, 17, 201-210.	5.3	16
77	Characterization of Perfluorooctylbromide-Based Nanoemulsion Particles Using Atomistic Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 10086-10096.	2.6	15
78	Nanoinformatics: developing new computing applications for nanomedicine. Computing (Vienna/New) Tj ETQq0 0 0 rgBT /Overlock 10 T	4.8	15
79	Understanding nucleic acid structural changes by comparing wide-angle x-ray scattering (WAXS) experiments to molecular dynamics simulations. Journal of Chemical Physics, 2016, 144, 205102.	3.0	15
80	SPrCY: comparison of structural predictions in the Saccharomyces cerevisiae genome. Bioinformatics, 2004, 20, 2312-2314.	4.1	14
81	Multi-shell model of ion-induced nucleic acid condensation. Journal of Chemical Physics, 2016, 144, 155101.	3.0	13
82	Atomic Radius and Charge Parameter Uncertainty in Biomolecular Solvation Energy Calculations. Journal of Chemical Theory and Computation, 2018, 14, 759-767.	5.3	13
83	Dynamical properties of fasciculin-2. , 1999, 36, 447-453.		12
84	Physicochemical signatures of nanoparticle-dependent complement activation. Computational Science & Discovery, 2014, 7, 015003.	1.5	12
85	Smoothed dissipative particle dynamics model for mesoscopic multiphase flows in the presence of thermal fluctuations. Physical Review E, 2016, 94, 023304.	2.1	11
86	Non-Boltzmann Rate Distributions in Stochastically Gated Reactions. Journal of Physical Chemistry B, 1999, 103, 615-617.	2.6	10
87	Electrostatic Interactions. Methods of Biochemical Analysis, 2005, , 427-440.	0.2	10
88	Bayesian model aggregation for ensembleâ€based estimates of protein pK_a values. Proteins: Structure, Function and Bioinformatics, 2014, 82, 354-363.	2.6	10
89	Nanoinformatics workshop report: current resources, community needs and the proposal of a collaborative framework for data sharing and information integration. Computational Science & Discovery, 2013, 6, 014008.	1.5	9
90	Numerical calculation of protein-ligand binding rates through solution of the Smoluchowski equation using smoothed particle hydrodynamics. BMC Biophysics, 2015, 8, 7.	4.4	9

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91	PBâ€AM: An openâ€source, fully analytical linear poissonâ€boltzmann solver. Journal of Computational Chemistry, 2017, 38, 1275-1282.	3.3	9
92	Origin of parameter degeneracy and molecular shape relationships in geometric-flow calculations of solvation free energies. Journal of Chemical Physics, 2013, 139, 204108.	3.0	8
93	Bayesian Model Averaging for Ensemble-Based Estimates of Solvation-Free Energies. Journal of Physical Chemistry B, 2017, 121, 3458-3472.	2.6	8
94	Structural phylogeny by profile extraction and multiple superimposition using electrostatic congruence as a discriminator. Intrinsically Disordered Proteins, 2013, 1, e25463.	1.9	7
95	A data-driven framework for sparsity-enhanced surrogates with arbitrary mutually dependent randomness. Computer Methods in Applied Mechanics and Engineering, 2019, 350, 199-227.	6.6	6
96	Ontologies for cancer nanotechnology research. , 2009, 2009, 4158-61.		5
97	Research towards a systematic signature discovery process. , 2013, , .		5
98	Domain-specific languages for composing signature discovery workflows. , 2012, , .		2
99	Energy Minimization of Discrete Protein Titration State Models Using Graph Theory. Journal of Physical Chemistry B, 2016, 120, 8354-8360.	2.6	2
100	Perturbation of Membrane Structure by Oxysterols. Biophysical Journal, 2010, 98, 491a.	0.5	1
101	Annotating the structure and components of a nanoparticle formulation using computable string expressions. , 2012, 2012, 889-894.		1
102	Improved Coarse-Grained Modeling of Cholesterol Activation in Lipid Bilayers. Biophysical Journal, 2013, 104, 590a-591a.	0.5	1
103	The Structural Basis of Cholesterol Accessibility in Membranes. Biophysical Journal, 2014, 106, 509a.	0.5	1
104	Adaptive visual sort and summary of micrographic images of nanoparticles for forensic analysis. , 2016, 2016, .		1
105	Weighted-Ensemble Brownian Dynamics for Charged Ligand Diffusion onto Acetylcholinesterase. , 1998, , 367-367.		1
106	Erratum to â€œProbing 3â€²-ssDNA Loop Formation in E. coli RecBCD/RecBCâ€“DNA Complexes Using Non-natural DNA: A Model for â€œChiâ€•Recognition Complexesâ€•[J. Mol. Biol. 359 (2006) 1137â€“1149]. Journal of Molecular Biology, 2007, 365, 900.	4.2	0
107	Communication Via Structural Water: Changes In The Thrombin Water Channel And Active Site Due To Sodium Binding. Biophysical Journal, 2009, 96, 595a-596a.	0.5	0
108	Multi-Scale Modeling of the â€œContact-Facilitatedâ€•Delivery Mechanism ofÂPerfluorocarbon-Based Nanoemulsions. Biophysical Journal, 2010, 98, 672a.	0.5	0

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109	Using physicochemical properties of amino acids to induce graphical models of residue couplings. , 2011, , .		0
110	APBSmem: A Tool for the Analysis of Membrane Protein Electrostatics. Biophysical Journal, 2012, 102, 682a.	0.5	0
111	Improving Implicit Solvent Models with Differential Geometry. Biophysical Journal, 2012, 102, 169a.	0.5	0
112	The Structural Basis of Cholesterol Activation in Membranes. Biophysical Journal, 2013, 104, 662a.	0.5	0
113	Informatics Approaches to Data Preservation and Analysis in Protein Electrostatics. Biophysical Journal, 2015, 108, 369a.	0.5	0
114	Condensation of Nucleic Acids by Multivalent Ions: Sequence Dependence and the Curious Case of RNA. Biophysical Journal, 2016, 110, 409a.	0.5	0
115	Mathematics and Molecular Neurobiology. Lecture Notes in Computational Science and Engineering, 2002, , 31-60.	0.3	0
116	Determining the mechanism of allosteric regulation of NikR binding to DNA activated by Ni ²⁺. FASEB Journal, 2006, 20, A489.	0.5	0
117	Molecular dynamics simulation of the NikR protein: Equilibrium conformational fluctuations reveal interâ€domain allosteric communication pathways. FASEB Journal, 2008, 22, 612.2.	0.5	0
118	Low-Barrier Hydrogen Bond in the Catalytic Triad of Serine Enzymes. , 1998, , 233-233.		0
119	A clustering-based biased Monte Carlo approach to protein titration curve prediction. , 2020, 2020, .		0